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FOODSIM'2010

FOODSIM 2010

BRAGANÇA, PORTUGAL · JUNE 24-26, 2010

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EDITED BY

VASCO CADAVEZ
AND
DANIEL THIEL

ORGANIZED BY



IN COOPERATION WITH



**6TH INTERNATIONAL CONFERENCE
ON
SIMULATION AND MODELLING
IN THE
FOOD AND BIO-INDUSTRY
2010**

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PREFACE

Dear colleagues,

Welcome to the 6th International Conference on Simulation and Modelling in Food and Bio Industries (FOODSIM'2010), which is held in Bragança, Portugal from 24 to 26 June 2010.

The FOODSIM'2010 brings together researchers, food experts and industrial users to present the state-of-art simulation research in the food industry, new research results and to exchange ideas and experiences about the modeling and simulation tools used in the food industry.

The main theme of FOODSIM'2010 is: "Simulation applied to food processes, quality, safety, and sustainability", and the success of the conference is already assured, as can be witnessed by the quality and scientific rigor of the 47 published papers. We also take this opportunity to challenge the researchers attending the FOODSIM'2010 to produce a seed for a FP7 project to be submitted at the next call for proposals, which is expected to open next July.

We present our recognition for the inestimable collaboration that we had in the FOODSIM'2010 organisation by Prof. Joana Amaral and Prof. Elsa Ramalhosa, and to all the reviewers for their professional work in the papers evaluation. We also present our recognition to all Institutions that contributed to prepare a pleasant social programme for FOODSIM'2010.

Finally, we wish you all a pleasant staying in Bragança and we are sure that you will have the opportunity to be delighted by the Portuguese hospitality.

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PHYSICAL CHARACTERISTICS AND DRYING KINETICS OF PORTUGUESE 'Longal' CHESTNUT

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KEYWORDS

Chestnut, Physical characteristics, Drying kinetics, Fick's second law, Apparent diffusivity.

ABSTRACT

Chestnut is a fruit of great importance in Portugal, being generally sold fresh or frozen. Alternative products may be obtained by hot air drying.

The present work is on the dehydration behavior of Portuguese 'Longal' chestnut, that is the most used in industry. Different models for representing the variations of water content and drying rate along time were tested successfully. As expected, higher temperatures correspond to faster drying processes. The apparent diffusivity was predicted by Fick's second law equation, and it ranged from $1.25 \times 10^{-11} \text{ m}^2/\text{s}$, at 20°C , to $8.42 \times 10^{-10} \text{ m}^2/\text{s}$, at 100°C .

INTRODUCTION

Chestnut (*Castanea sativa*) has always been used in human feeding. Nowadays, chestnuts have high economic importance in Portugal because this country is an important exporter of this fruit, contributing significantly to the equilibrium of Portuguese commercial balance. Chestnut production is more significant in the North of Portugal, namely in Trás-os-Montes and Beiras regions, reaching the highest commercial values and representing 86% of the national production (INE 2008). In 2007, for example, 7 774 ton of chestnut were exported, originating €14 844 000.

Portuguese varieties of chestnut are of excellent quality. Three Protected Origin Denominations have been identified, namely Chestnut of Terra Fria, Chestnut of Soutos da Lapa and Chestnut of Padrela. Being a seasonal product, the chestnut needs to be preserved in order to be sold as a fresh produce, or to be further processed. Traditionally, chestnuts are left in warehouses at room

temperature, being consumed along the year by the local families. This chestnut is known as "castanha pilada", being dehydrated and extremely sweet. On the contrary, in industry chestnuts are stored under refrigeration until their sale as fresh produce, or they are frozen after peeling.

In industrial chestnut preservation, two main problems have been detected. These are related to weight losses (due to dehydration of the fresh chestnut) and to the development of microorganisms, namely fungi producers of micotoxins, such as aflatoxins, which present an eminent danger for public health, as the latter are considered carcinogenic, hepatotoxic, and teratogenic. Besides, there is a need of finding alternatives for chestnuts with low quality to the final consumers, such as small fruits, that are often discarded, and of developing innovative products based on chestnut, allowing the diversification of products and the development of others able to be incorporated into a wide variety of food stuffs, such as chestnut flour. Therefore, it is of great importance to find alternative preservation and processing technologies.

Taking into account the popular knowledge, the dehydration of chestnut seems to be a promising technology, as chestnuts could be stored for longer periods without the problem of fungi development. Recently, some interesting studies on drying of chestnut have been performed, involving New Zealand (Cletus and Carson 2008), Italian (Attanasio et al. 2004), Turkish (Koyuncu et al. 2004) and even Portuguese (Guiné and Fernandes 2006) varieties. In relation to this last work, three Portuguese varieties were analyzed, namely 'Longal', 'Martainha' and 'Viana', which were subjected to three drying temperatures; 70, 80 and 90°C . The first two varieties showed better drying features than the last. Nevertheless, the use of lower temperatures may also be promising. Moreover, variability of the characteristics of chestnuts harvested in different

years might have an important role on their drying behaviour and be a factor that must be taken into account. In fact, chestnut producers refer that the year 2009 was not a good year for chestnut production, due to the lack of water during the maturation stage, originating small fruits.

Taking into account these aspects, the aims of this work were: i) to determine some physical properties of 'Longal' chestnuts, which is one of the most used in industry (due to the easiness of peeling and to the pulp not being too sectioned), collected in the year 2009; ii) to study and find empirical models that will allow the estimation of the drying rates of these chestnuts when subjected to different drying temperatures (20, 40, 50, 65, 85 and 100°C); iii) to evaluate the effect of drying on chestnuts dimensions; iv) to evaluate the adequacy of the Fick's second law to express the drying process; v) to estimate the apparent diffusivity of water in this Portuguese chestnut variety.

MATERIALS AND METHODS

Portuguese 'Longal' chestnuts were supplied by a local producer of Trás-os-Montes region, North of Portugal, being harvested in November 2009. When arriving to the laboratory, chestnuts were carefully observed and the ones that were rotten were discarded.

Chestnuts were individually weighed and their ellipsoid axis dimensions (a : length; b : width; c : thickness) determined. To perform the drying experiments, chestnuts were placed in a convection oven (Binder, Germany) at 40, 50, 65, 85 and 100°C. To perform the assay at 20°C, chestnuts were left at room temperature. In each experiment, chestnuts were put inside the oven in several Petri dishes. Each Petri dish contained 5 chestnuts. One Petri dish was removed at defined time moments, the fruits being analyzed again (weight and ellipsoid axis dimensions) with and without outer peel, in order to evaluate the shrinkage.

At the beginning of each experiment, the dry matter content of the chestnuts used in the assay was determined by drying five chestnuts at 105°C until the sample weight reached a steady value. The dry-basis moisture content (W , kg of water/ kg of dry matter) was determined for each chestnut. At each time moment, the average, standard deviation and coefficient of variation were determined for the five chestnuts removed.

In order to evaluate the suitability of approaching the chestnuts to spheres in the diffusion equation, the diameter of chestnuts was determined after immersion of twenty chestnuts in water and measurement of the volume of water displaced. These values were later compared with the arithmetic (D_a) and geometric (D_g) average diameters determined by equations (1) and (2), respectively (Mohsenin 1970; Güner 2007; Kılıçkan and Güner 2008):

$$D_a = \frac{a+b+c}{3} \quad (1)$$

$$D_g = \sqrt[3]{a \times b \times c} \quad (2)$$

Chestnut sphericity (ϕ) was also evaluated by equation (3) (Mohsenin 1970; Güner 2007; Kılıçkan and Güner 2008):

$$\phi = \frac{\sqrt[3]{a \times b \times c}}{b} \quad (3)$$

, considering b the biggest dimension.

DRYING CURVES COMPUTER FITTING

For all the assays, the drying curves (W versus time) followed a similar pattern, expressed by an exponential function of the form:

$$W = y + A \times e^{(-kt)} \quad (4)$$

where y , A and k were parameters of the model.

In order to determine the drying rates $\left(\frac{\partial W}{\partial t}\right)$, the method of the approximation of the derivative to finite differences was used (Guiné and Fernandes 2006):

For $t=t_0$

$$\left(\frac{\partial W}{\partial t}\right) = \frac{W_1 - W_0}{t_1 - t_0} \quad (\text{first-order forward finite differences}) \quad (5)$$

For $t=t_i$ ($i = 1, \dots, N-1$)

$$\left(\frac{\partial W}{\partial t}\right) = \frac{W_{i+1} - W_{i-1}}{t_{i+1} - t_{i-1}} \quad (\text{second-order centred finite differences}) \quad (6)$$

For $t=t_N$

$$\left(\frac{\partial W}{\partial t}\right) = \frac{W_N - W_{N-1}}{t_N - t_{N-1}} \quad (\text{first-order backward finite differences}) \quad (7)$$

A linear and a sigmoid function (Eq. 8) were used to express the relationship encountered between the drying rate and the moisture content.

$$-\left(\frac{\partial W}{\partial t}\right) = y + \frac{A}{1 + e^{\left(\frac{C-W}{B}\right)}} \quad (8)$$

All the models presented, with exception of the linear, were obtained after using the non-linear regression of the SPSS software package.

The quality of all models was evaluated by the correlation coefficient (r), reduced chi-square (χ^2), mean bias error (MBE) and root mean square error (RMSE) (Guiné and Fernandes 2006), determined by the following equations:

$$\chi^2 = \frac{1}{N-n} \sum_{i=1}^N (V_{\text{exp},i} - V_{\text{pred},i})^2 \quad (9)$$

$$MBE = \frac{1}{N} \sum_{i=1}^N (V_{\text{pred},i} - V_{\text{exp},i}) \quad (10)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (V_{\text{pred},i} - V_{\text{exp},i})^2} \quad (11)$$

where $V_{\text{exp},i}$ and $V_{\text{pred},i}$ are the experimental and predicted values for the observation i ; N is the number of observations; and n the number of parameters in the model. The higher the value of “ r ” and the lower the values of χ^2 , MBE and RMSE, the better the model fitted the experimental results.

RESULTS AND DISCUSSION

Physical Properties of Portuguese ‘Longal’ Chestnuts

Table 1 shows some physical properties of the ‘Longal’ chestnuts used in all drying assays. The dimensions of ellipsoid axis of chestnuts (a , b , c) varied within the ranges of 2.62-2.82, 3.10-3.29 and 1.69-1.91 cm, respectively, corresponding to variation coefficients less than 7.9, 6.4 and 16.4%. The arithmetic and geometric mean diameters of chestnuts varied between 2.47-2.66 and 2.39-2.58 cm, respectively, corresponding to variation coefficients less than 6.3 and 7.1%, respectively. The low values obtained for the variation coefficients, with the exception of dimension c , that was the most difficult to measure, are indicative of the existence of homogeneity among the chestnuts used in all assays.

In terms of chestnut sphericity, this parameter varied within the range of 76.9 to 79.2%, indicating that chestnuts might be approximated to spheres.

When comparing the diameter (D , results not shown) determined by immersion in water (considering chestnuts as spheres) with D_a or D_g , determined by equations (12) and (13), respectively, linear relationships were encountered between both parameters, namely:

$$D_a = 0.7707 \times D + 0.7304 \quad (r=0.922) \quad (12)$$

$$D_g = 0.8139 \times D + 0.5451 \quad (r=0.916) \quad (13)$$

These results indicate that either D_g or D_a may be used to estimate the diameter of ‘Longal’ chestnuts when it is intended to approach them as spheres.

Drying curves of Portuguese ‘Longal’ chestnuts

The experimental points determined along the drying of ‘Longal’ chestnuts at 20, 40, 50, 65, 85 and 100°C are in Figure 1. In each graph the predicted points obtained in the fits by using Eq. 4 are also presented, as well as the model equation and the correlation coefficient.

Figure 1 shows that the fits to the experimental data at 20, 40, 50, 65, 85 and 100°C are good, with correlation coefficients ranging from 0.989 to 0.998. The χ^2 , MBE and RMSE values were also low, varying between 3.05×10^{-4} and 9.87×10^{-4} , -6.77×10^{-4} and 1.69×10^{-2} , and 1.59×10^{-2} and 2.79×10^{-2} , respectively.

The drying rate values determined by derivation of Eq. 4 are in Figure 2, with correlation coefficients ranging from 0.863 to 0.969. The quality of the model is quite good taking into account the similarity with the experimental data, and the χ^2 , MBE and RMSE values, which were low, between 5.43×10^{-8} and 5.28×10^{-4} , -2.49×10^{-5} and 3.71×10^{-3} , 2.21×10^{-4} and 2.07×10^{-2} , respectively.

By observing the drying rate curves obtained, no constant rate period was observed (Figure 2). Higher temperatures corresponded to faster drying processes, which is reflected on the increasing dehydration constants: 0.003 for 20°C, 0.019 for 40°C, 0.029 for 50°C, 0.062 for 65°C, 0.142 for 85°C, and 0.189 for 100°C.

In terms of the relation between drying rate curves and moisture content, both linear and sigmoidal (Eq. 8) functions seem to represent well the experimental data (Table 2). The correlation coefficients of both models varied between 0.902-0.956 and 0.927-0.967, respectively. The χ^2 , MBE and RMSE values were low again, varying between 5.27×10^{-8} and 3.86×10^{-4} , -2.57×10^{-5} and 1.86×10^{-3} ,

and 2.17×10^{-4} and 1.77×10^{-2} , for the linear model, and between 4.09×10^{-6} and 2.76×10^{-4} , -1.30×10^{-4} and 1.50×10^{-3} , and 1.84×10^{-3} and 1.50×10^{-2} , for sigmoidal model, respectively.

Table 1: Physical properties of ‘Longal’ chestnuts used in the drying assays¹.

Temperature of the assay (°C)	<i>a</i> (cm)	<i>b</i> (cm)	<i>c</i> (cm)	<i>D_a</i> (cm)	<i>D_g</i> (cm)	<i>ϕ</i> (%)
20	2.75±0.20	3.20±0.15	1.71±0.28	2.55±0.15	2.46±0.17	76.9±6.0
40	2.72±0.20	3.23±0.19	1.86±0.27	2.60±0.16	2.53±0.18	78.5±4.4
50	2.62±0.17	3.10±0.16	1.69±0.22	2.47±0.12	2.39±0.13	77.1±4.1
65	2.76±0.20	3.26±0.21	1.91±0.27	2.64±0.15	2.57±0.16	79.2±4.6
85	2.67±0.21	3.16±0.18	1.74±0.24	2.53±0.16	2.45±0.17	77.4±4.0
100	2.82±0.17	3.29±0.17	1.88±0.29	2.66±0.15	2.58±0.16	78.7±4.6

¹ Results are the averages of the determinations ± Standard deviation.

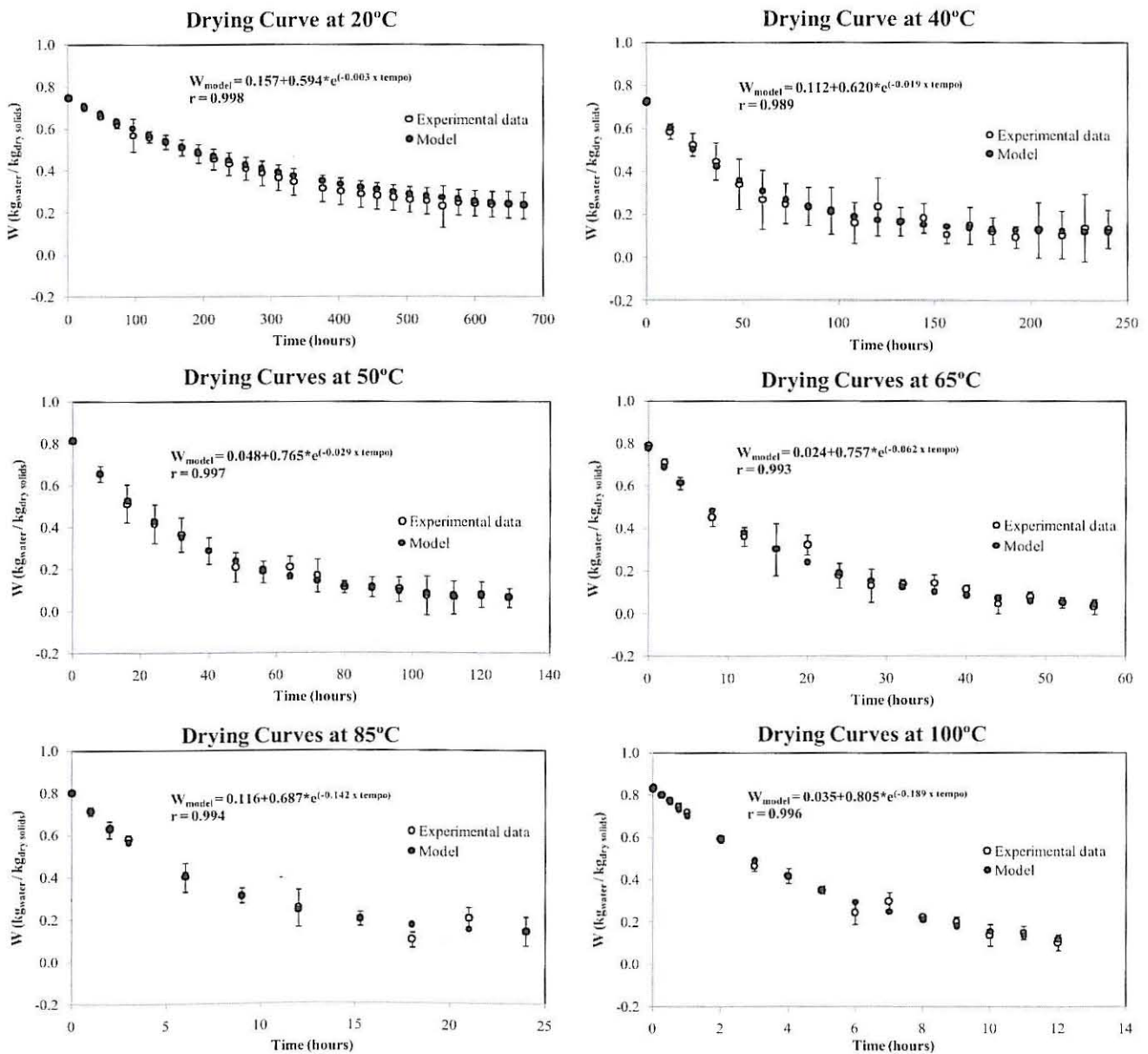


Figure 1: Drying data of ‘Longal’ chestnuts at 20, 40, 50, 65, 85 and 100°C.

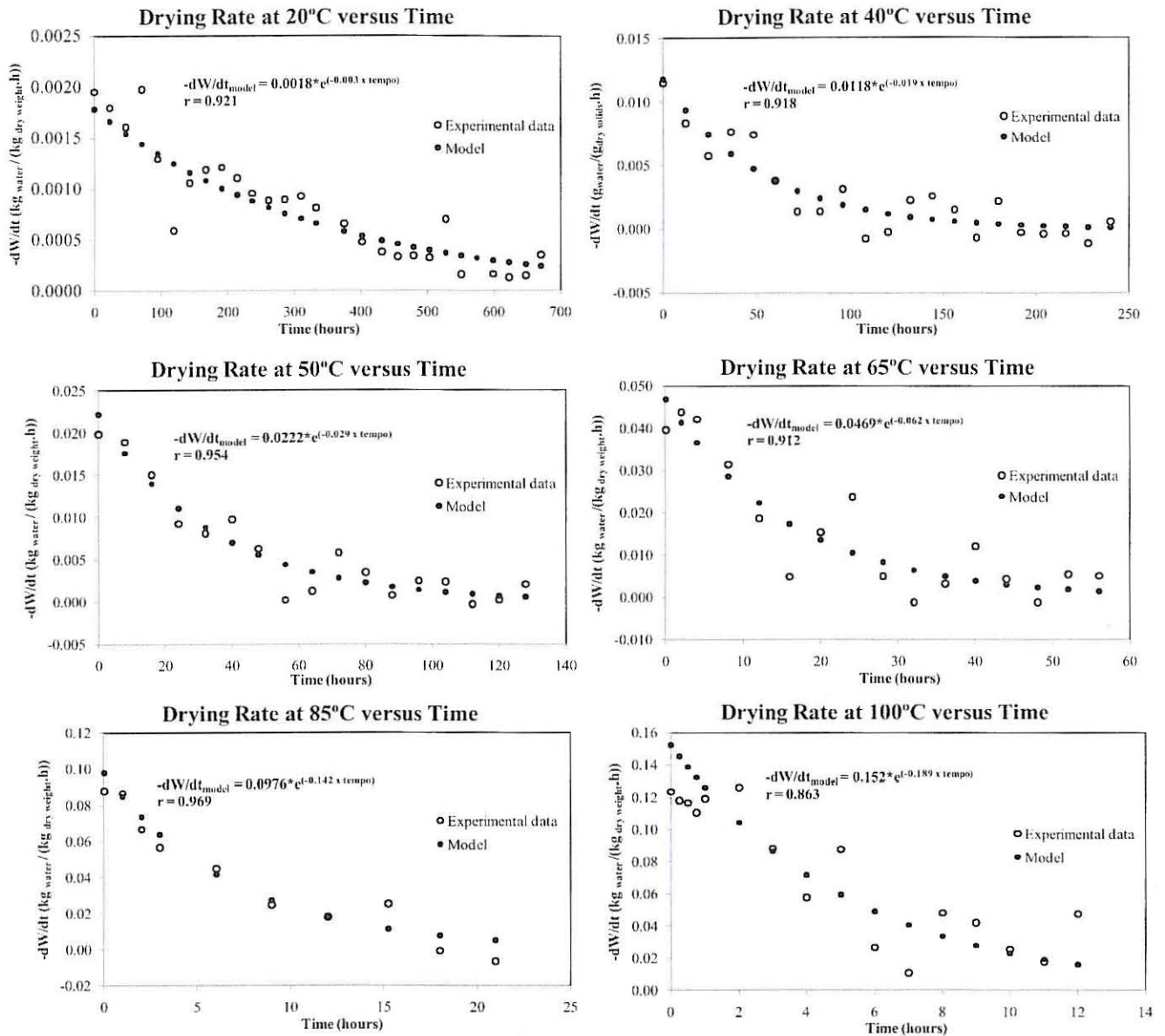


Figure 2: Drying rates of 'Longal' chestnuts at 20, 40, 50, 65, 85 and 100°C.

Table 2: Linear and sigmoidal models for the drying rates in function of moisture content.

Model	T(°C)	Model Parameters	Correlation Coefficient (r)
Linear model $-\left(\frac{\partial W}{\partial t}\right) = A + B \times W$	20	A = -0.0005; B = 0.0032	0.924
	40	A = -0.002; B = 0.0183	0.908
	50	A = -0.0011; B = 0.0277	0.952
	65	A = -0.0004; B = 0.058	0.906
	85	A = -0.0114; B = 0.1266	0.956
	100	A = 0.0089; B = 0.1447	0.902
Sigmoidal model (Eq. 8) $-\left(\frac{\partial W}{\partial t}\right) = y + \frac{A}{1 + e^{\left(\frac{C-W}{B}\right)}}$	20	Not adequate	--
	40	Not adequate	--
	50	y = -0.001; A = 0.023; B = 0.158; C = 0.402	0.957
	65	y = 0.006; A = 0.037; B = 0.059; C = 0.400	0.930
	85	y = -32.935; A = 33.963; B = 7.167; C = -24.724	0.967
	100	y = 0.034; A = 0.086; B = 0.059; C = 0.427	0.927

Evaluation of the effect of drying on chestnuts dimensions

Drying at 40, 50, 65, 85 and 100°C did not cause significant changes in chestnuts dimensions, indicating that the effect of shrinkage may be neglected. In fact, the average geometric diameters of the chestnuts were identical at the beginning and at the end of all assays (Table 3). Even at high temperatures no significant reduction on chestnuts size was detected. Moreover, the fruit without outer shell after drying corresponded always to 76.5 – 80.2% of the fruit with outer shell, no differences being detected among drying experiments at different temperatures.

Evaluation of the adequacy of Fick's second law to the drying process

Assuming that chestnuts may be approximated to spheres, and considering that the drying rate depends solely on the moisture movement by diffusion within the chestnut, the process might be represented by the following Fick's second law equation for non-steady state:

$$\frac{\partial W}{\partial t} = D_{ap} \left(\frac{\partial^2 W}{\partial r^2} + \frac{2}{r} \times \frac{\partial W}{\partial r} \right) \quad (14)$$

where D_{ap} is the apparent diffusivity, r is the radius and t is time. Assuming uniform initial moisture content (W_0) and that the internal mass transfer resistance is controlling over external resistance, the analytical solution of Eq. 14 is the following:

$$\frac{W - W_e}{W_0 - W_e} = \frac{6}{\pi^2} \sum_{i=1}^{\infty} \frac{1}{n^2} \exp\left(-D_{ap} \frac{n^2 \pi^2}{R^2} t\right) \quad (15)$$

where W_e is the equilibrium dry-basis moisture content.

Considering that only the first term is significant and W_e may be estimated by Eq. 4 for $t \rightarrow \infty$ ($W_e = y$), taking the natural logarithm of each side of Eq. 15, the following linear equation will be obtained:

$$\ln\left(\frac{W - W_e}{W_0 - W_e}\right) = \ln\frac{6}{\pi^2} - D_{ap} \frac{\pi^2}{R^2} t \quad (16)$$

Fitting the data by Eq. 16, linear correlations were obtained (Figure 3), with coefficient correlations ranging between 0.947 and 1.000. These results indicate that the assumptions assumed seem to be adequate.

Estimation of the apparent diffusivities of 'Longal' chestnut variety

Taking into account Eq.16, the apparent diffusivities of *Longal* chestnut may be determined by the following equation:

$$D_{ap} = -\frac{slope \times R^2}{\pi^2} \quad (17)$$

Considering the slope for each temperature (Figure 3) and the average radius of the chestnuts, based either on D_g or D_a , used in each assay, the apparent diffusivities obtained for 'Longal' chestnut are in Table 4.

Table 4: Apparent diffusivities of water in 'Longal' chestnut.

Temperature (°C)	D_{ap} (m ² /s)
20	1.25×10^{-11}
40	6.53×10^{-11}
50	1.08×10^{-10}
65	2.89×10^{-10}
85	5.24×10^{-10}
100	8.42×10^{-10}

When comparing these values with the ones reported by Guiné and Fernandes (2006) for the same chestnut variety dried at 70-90°C (4.45×10^{-9} to 6.87×10^{-9} m²/s), the present results are one order of magnitude lower. This might be related to the worse quality of the chestnuts used in the assays, as the year 2009 was not adequate for a good quality of the nuts. So, in the future it would be interesting to study the role of the harvest year on the drying characteristics of chestnuts. However, the results determined at 20-40°C (1.25×10^{-11} to 6.53×10^{-11} m²/s) are in accordance to the one determined for the New Zealand chestnut variety "1015" at 30°C (Cletus and Carson 2008), namely 5.1×10^{-11} m²/s.

Table 3: Average geometric diameters of chestnuts determined before and after the drying assays.

Temperature (°C)	D _g initial (with outer peel)	D _g final (with outer peel)	D _g final (without outer peel)	D _g final (without outer peel) / D _g final (with outer peel) (%)
40	2.50±0.22	2.45 ± 0.19	1.93 ± 0.22	78.8
50	2.40 ± 0.13	2.34 ± 0.11	1.79 ± 0.14	76.5
65	2.50 ± 0.19	2.40 ± 0.18	1.91 ± 0.15	79.6
85	2.39 ± 0.22	2.32 ± 0.23	1.86 ± 0.21	80.2
100	2.54 ± 0.10	2.43 ± 0.09	1.89 ± 0.10	77.8

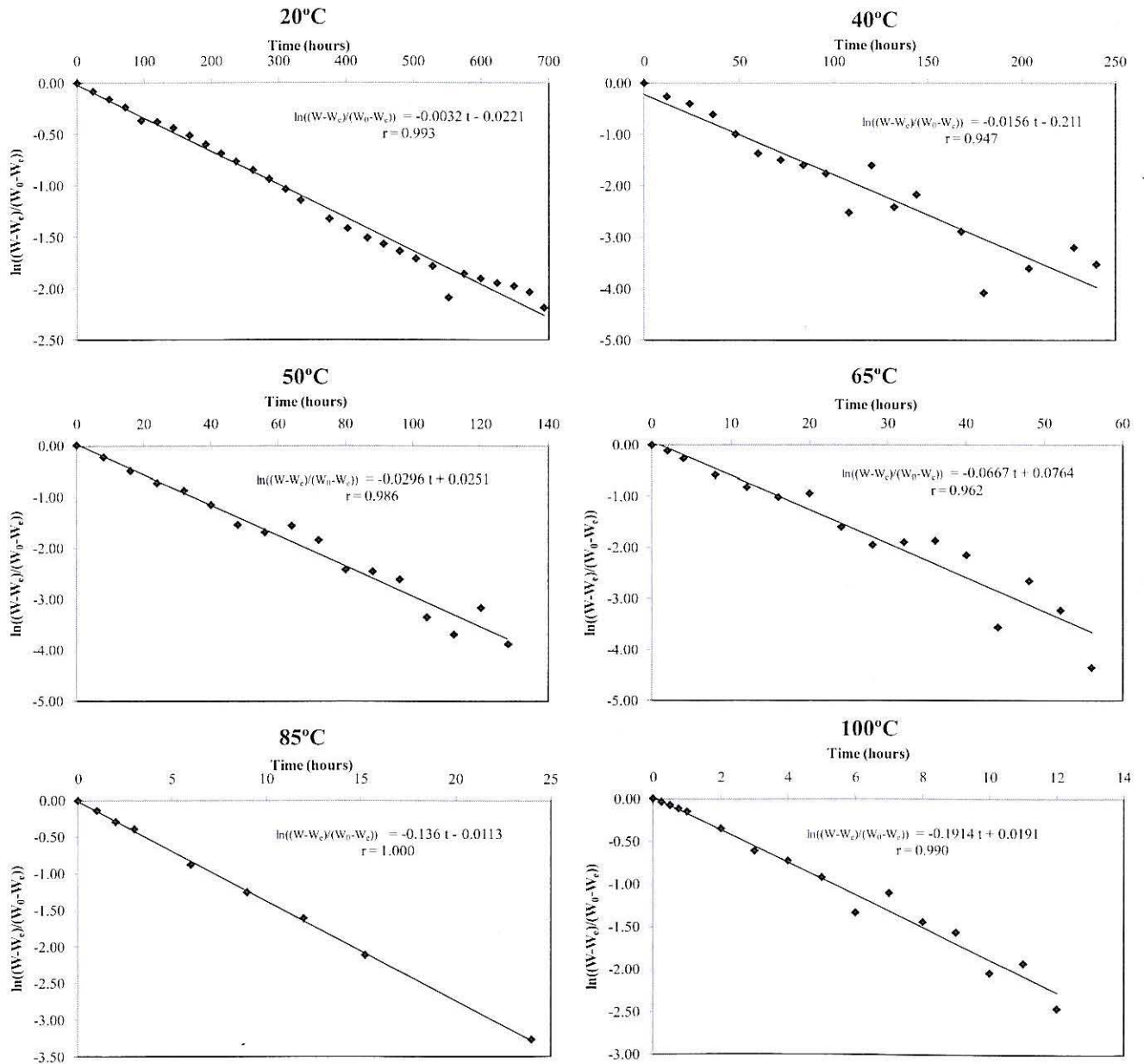


Figure 3: $\ln((W-W_e)/(W_0-W_e))$ versus time for the drying assays at 20, 40, 50, 65, 85 and 100°C.

CONCLUSIONS

There was homogeneity among the chestnuts used in the drying experiments. An exponential empirical model fitted well the experimental drying data for several temperatures between 20°C and 100°C. Linear and sigmoid functions also fitted well the drying experimental rates. Approximating chestnuts (sphericity being higher than 77%) to spheres, the apparent diffusivity predicted by Fick's second law was between 1.25×10^{-11} m²/s, at 20°C, to 8.42×10^{-10} m²/s, at 100°C.

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